

Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt
946-30-5 | DTXSID4061339

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.69

Global applicability domain: Inside

Local applicability domain index: 6.88e-01

Confidence level: 3.72e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Phenacetin</div> <div>Measured: 9.59</div> <div>Predicted: 9.23</div>	<div>Image not found</div> <div>Diphenylamine</div> <div>Measured: 7.64</div> <div>Predicted: 8.73</div>	<div>Image not found</div> <div>1-Hexadecanol</div> <div>Measured: 9.90</div> <div>Predicted: 9.79</div>
<div>Image not found</div> <div>Methylparaben</div> <div>Measured: 8.57</div> <div>Predicted: 7.06</div>	<div>Image not found</div> <div>1-Octanol</div> <div>Measured: 6.03</div> <div>Predicted: 5.95</div>	